(Time-dependent) Mean-field approaches to nuclear response and reaction

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    - HFBTHO(2D)+FAM (2D HO-basis rep.)
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  - Shell effects/Magic numbers/Neutron skin
- Glauber calculation of reaction cross section
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Time-dependent Hartree-Fock (TDHF)

Time-dependent Hartree-Fock equation

$$i\frac{\partial}{\partial t}\phi_i(t) = \left\{h(t) + V_{\text{ext}}(t)\right\}\phi_i(t)$$

$$i\frac{\partial}{\partial t}\rho(t) = \left[h(t) + V_{\text{ext}}(t), \rho(t)\right]$$

$$\rho(\vec{r}, t) = \sum_{i=1}^{N} \left|\phi_i(\vec{r}, t)\right|^2$$

$$h(t) = h\left[\rho(t)\right]$$

TDHFB for superfluid systems

Time-dependent Hartree-Fock-Bogoliubov equation

$$\boxed{\begin{aligned} i\frac{\partial}{\partial t}\Psi_i(t) &= \{H(t)+V_{\text{ext}}(t)\}\Psi_i(t) \\ i\frac{\partial}{\partial t}R(t) &= [H(t)+V_{\text{ext}}(t), R(t)] \end{aligned}}$$

$$\Psi_i = \begin{pmatrix} U_i \\ V_i \end{pmatrix} \qquad H(t) = H[R(t)] = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}$$

$$R(t) = \sum_i \Psi_i \Psi_i^+ = \begin{pmatrix} \rho(t) & \kappa(t) \\ -\kappa^*(t) & 1-\rho^*(t) \end{pmatrix}$$

Small-amplitude limit
(Random-phase approximation)

One-body density operator under a TD external potential

$$i\frac{\partial}{\partial t}\rho(t) = \left[h(t) + V_{\mathrm{ext}}(t), \rho(t)\right]$$

Assuming that the external potential is weak,

$$\rho(t) = \rho_0 + \delta\rho(t) \qquad h(t) = h_0 + \delta h(t) = h_0 + \left.\frac{\delta h}{\delta\rho}\right|_{\rho_0} \cdot \delta\rho(t)$$

$$i\frac{\partial}{\partial t}\delta\rho(t) = \left[h_0, \delta\rho(t)\right] + \left[\delta h(t) + V_{\mathrm{ext}}(t), \rho_0\right]$$

Let us take the external field with a fixed frequency ω,

$$V_{\mathrm{ext}}(t) = V_{\mathrm{ext}}(\omega)e^{-i\omega t} + V_{\mathrm{ext}}^{+}(\omega)e^{+i\omega t}$$

The density and residual field also oscillate with ω,

$$\delta\rho(t) = \delta\rho(\omega)e^{-i\omega t} + \delta\rho^{+}(\omega)e^{+i\omega t}$$

$$\delta h(t) = \delta h(\omega)e^{-i\omega t} + \delta h^{+}(\omega)e^{+i\omega t}$$

The linear response (RPA) equation

$$\omega\delta\rho(\omega) = \left[h_0, \delta\rho(\omega)\right] + \left[\delta h(\omega) + V_{\rm ext}(\omega), \rho_0\right]$$

Note that all the quantities, except for ρ_0 and h_0, are non-hermitian.

$$\delta\rho(t) = \sum_{i=1}^{A}\left(\left|\delta\psi_i(t)\right\rangle\left\langle\phi_i\right| + \left|\phi_i\right\rangle\left\langle\delta\psi_i(t)\right|\right)$$

$$\Rightarrow \qquad \delta\rho(\omega) = \sum_{i=1}^{A}\left(\left|X_i(\omega)\right\rangle\left\langle\phi_i\right| + \left|\phi_i\right\rangle\left\langle Y_i(\omega)\right|\right)$$

This leads to the following equations for X and Y:

$$\omega\left|X_i(\omega)\right\rangle = \left(h_0 - \varepsilon_i\right)\left|X_i(\omega)\right\rangle + \hat{Q}\left\{\delta h(\omega) + V_{\rm ext}(\omega)\right\}\left|\phi_i\right\rangle$$

$$\omega\left\langle Y_i(\omega)\right| = -\left\langle Y_i(\omega)\right|\left(h_0 - \varepsilon_i\right) - \left\langle\phi_i\right|\left\{\delta h(\omega) + V_{\rm ext}(\omega)\right\}\hat{Q}$$

$$\hat{Q} = \sum_{i=1}^{A}\left(1 - \left|\phi_i\right\rangle\left\langle\phi_i\right|\right)$$

These are nothing but the “RPA linear-response equations”.
X and Y are called “forward” and “backward” amplitudes.

Matrix formulation

$$\omega\left|X_i(\omega)\right\rangle = \left(h_0-\varepsilon_i\right)\left|X_i(\omega)\right\rangle + \hat{Q}\left\{\delta h(\omega)+V_{\rm ext}(\omega)\right\}\left|\phi_i\right\rangle$$
$$\omega\left\langle Y_i(\omega)\right| = -\left\langle Y_i(\omega)\right|\left(h_0-\varepsilon_i\right) - \left\langle\phi_i\right|\left\{\delta h(\omega)+V_{\rm ext}(\omega)\right\}\hat{Q} \qquad (1)$$

$$\hat{Q} = 1-\sum_{i=1}^{A}\left|\phi_i\right\rangle\left\langle\phi_i\right|$$

If we expand the X and Y in *particle orbitals*:

$$\left|X_i(\omega)\right\rangle = \sum_{m>A}\left|\phi_m\right\rangle X_{mi}(\omega)\,,\quad \left|Y_i(\omega)\right\rangle = \sum_{m>A}\left|\phi_m\right\rangle Y_{mi}^*(\omega)$$

Taking overlaps of Eq.(1) with particle orbitals

$$\left\{\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\}\begin{pmatrix} X_{mi}(\omega) \\ Y_{mi}(\omega) \end{pmatrix} = -\begin{pmatrix} (V_{\rm ext})_{mi} \\ (V_{\rm ext})_{im} \end{pmatrix}$$

$$A_{mi,nj} = (\varepsilon_m-\varepsilon)\delta_{mn}\delta_{ij} + \left\langle\phi_m\right|\left.\frac{\partial h}{\partial\rho_{nj}}\right|_{\rho_0}\left|\phi_i\right\rangle$$

$$B_{mi,nj} = \left\langle\phi_m\right|\left.\frac{\partial h}{\partial\rho_{jn}}\right|_{\rho_0}\left|\phi_i\right\rangle$$

In many cases, setting $V_{\rm ext}$=0 and solve the normal modes of excitations:
→ Diagonalization of the matrix

Small-amplitude approximation
--- Linear response (RPA) equation ---

$$\left\{\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\}\begin{pmatrix} X_{mi}(\omega) \\ Y_{mi}(\omega) \end{pmatrix} = -\begin{pmatrix} (V_{\text{ext}})_{mi} \\ (V_{\text{ext}})_{im} \end{pmatrix}$$

$$A_{mi,nj} = (\varepsilon_m - \varepsilon)\delta_{mn}\delta_{ij} + \boxed{\left\langle \phi_m \left| \frac{\partial h}{\partial \rho_{nj}}\right|_{\rho_0} \right| \phi_i \right\rangle}$$

$$B_{mi,nj} = \boxed{\left\langle \phi_m \left| \frac{\partial h}{\partial \rho_{jn}}\right|_{\rho_0} \right| \phi_i \right\rangle}$$

- Tedious calculation of residual interactions
- Computationally very demanding, especially for deformed systems.

However, in principle, the self-consistent single-particle Hamiltonian should contain everything. We can avoid explicit calculation of residual interactions.

Finite Amplitude Method

T.N., Inakura, Yabana, PRC76 (2007) 024318.

Residual fields can be estimated by the finite difference method:

$$\delta h(\omega) = \frac{1}{\eta}\left(h\left[\langle\psi'|,|\psi\rangle\right] - h_0\right)$$

$$|\psi_i\rangle = |\phi_i\rangle + \eta|X_i(\omega)\rangle, \quad \langle\psi_i'| = \langle\phi_i| + \eta\langle Y_i(\omega)|$$

Starting from initial amplitudes $X^{(0)}$ and $Y^{(0)}$, one can use an iterative method to solve the following linear-response equations.

$$\omega|X_i(\omega)\rangle = (h_0 - \varepsilon_i)|X_i(\omega)\rangle + \hat{Q}\{\delta h(\omega) + V_{\mathrm{ext}}(\omega)\}|\phi_i\rangle$$

$$\omega\langle Y_i(\omega)| = -\langle Y_i(\omega)|(h_0 - \varepsilon_i) - \langle\phi_i|\{\delta h(\omega) + V_{\mathrm{ext}}(\omega)\}\hat{Q}$$

Programming of the RPA code becomes very much trivial, because we only need calculation of the single-particle potential, with different bras and kets.

Step-by-step numerical procedure

1. Set the initial amplitudes $X^{(0)}$ and $Y^{(0)}$
2. Calculate the residual fields δ h by the FAM formula

$$\delta h(\omega) = \frac{1}{\eta}\left(h\left[\langle\psi'|, |\psi\rangle\right] - h_0\right)$$

$$|\psi_i\rangle = |\phi_i\rangle + \eta |X_i(\omega)\rangle, \quad \langle\psi_i'| = \langle\phi_i| + \eta\langle Y_i(\omega)|$$

3. Now, we can calculate the l.h.s. of the following equations:

$$\left.\begin{aligned} &(\omega - h_0 + \varepsilon_i)|X_i(\omega)\rangle - \delta h(\omega)|\phi_i\rangle = V_{\text{ext}}(\omega)|\phi_i\rangle \\ &\langle Y_i(\omega)|(\omega + h_0 - \varepsilon_i) + \langle\phi_i|\delta h(\omega) = -\langle\phi_i|V_{\text{ext}}(\omega) \end{aligned}\right\} \Rightarrow A\vec{x} = \vec{b}$$

$$\vec{x} = \begin{pmatrix} |X_i(\omega)\rangle \\ \langle Y_i(\omega)| \end{pmatrix}, \quad \vec{b} = \begin{pmatrix} V_{\text{ext}}(\omega)|\phi_i\rangle \\ -\langle\phi_i|V_{\text{ext}}(\omega) \end{pmatrix}$$

4. Update the amplitude to $(X^{(1)},Y^{(1)})$ by an iterative algorithm, such as the conjugate gradient method and its derivatives

TDHFB for superfluid systems

Time-dependent Hartree-Fock-Bogoliubov equation

$$\boxed{\begin{aligned} i\frac{\partial}{\partial t}\Psi_i(t) &= \left\{H(t)+V_{\text{ext}}(t)\right\}\Psi_i(t) \\ i\frac{\partial}{\partial t}R(t) &= \left[H(t)+V_{\text{ext}}(t), R(t)\right] \end{aligned}}$$

$$\Psi_i = \begin{pmatrix} U_i \\ V_i \end{pmatrix} \qquad H(t) = H\left[R(t)\right] = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}$$

$$R(t) = \sum_i \Psi_i \Psi_i^+ = \begin{pmatrix} \rho(t) & \kappa(t) \\ -\kappa^*(t) & 1-\rho^*(t) \end{pmatrix}$$

Finite amplitude method for superfluid systems

Avogadro and TN, PRC **84**, 014314 (2011)

Residual fields can be calculated by

$$\delta h(\omega) = \frac{1}{\eta}\left\{h\left[\overline{V}_\eta^*, V_\eta\right] - h_0\right\}$$

$$\delta\Delta(\omega) = \frac{1}{\eta}\left\{\Delta\left[\overline{V}_\eta^*, U_\eta\right] - \Delta_0\right\}$$

$$V_\eta = V + \eta U^* Y, \quad \overline{V}_\eta^* = V^* + \eta U X$$

$$U_\eta = U + \eta V^* Y$$

QRPA equations are

$$(E_\mu + E_\nu - \omega) X_{\mu\nu} + \delta H_{\mu\nu}^{20} = F_{\mu\nu}^{20}$$

$$(E_\mu + E_\nu + \omega) Y_{\mu\nu} + \delta \widetilde{H}_{\mu\nu}^{02*} = F_{\mu\nu}^{02}$$

$$\begin{pmatrix} & \delta H_{\mu\nu} \\ \delta\widetilde{H}_{\mu\nu} & \end{pmatrix} = W^+ \begin{pmatrix} \delta h & \delta\Delta \\ \delta\widetilde{\Delta}^+ & -\delta h^+ \end{pmatrix} W$$

$$W = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}$$

Implementation of the Finite amplitude method

- (TD)HF (3D coord.) + FAM
  - Implementation by Tsunenori Inakura
  - Inakura, T.N., Yabana, PRC **80**, 044301 (2009); arXiv:1106.3618
- Spherical HFB (radial coord.) + FAM
  - Implementation to HFBRAD by Paolo Avogadro
  - Time-odd fields are added
  - Avogadro and T.N., PRC **84**, 014314 (2011)
- Deformed HFB + FAM
  - Implementation to HFBTHO by Mario & Markus
  - Time-odd fields are added
  - Stoitsov et al, arXiv:1107.3530

HFBRAD+FAM

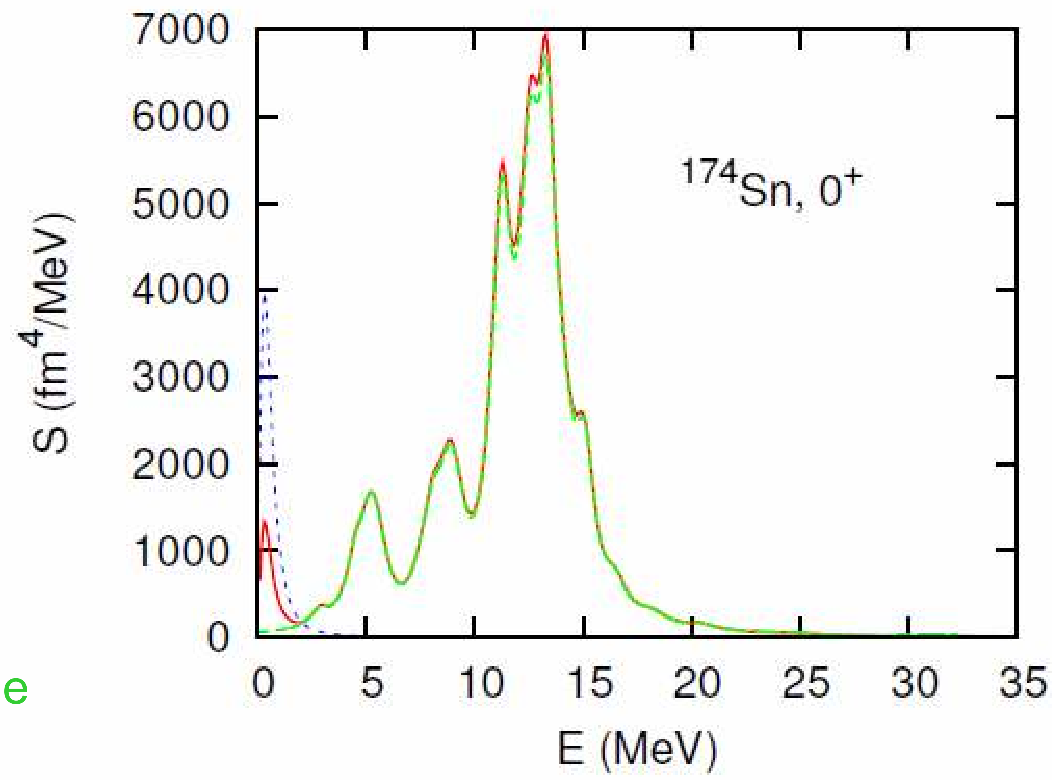
Test calculation: IS monopole

Our result: Red line

qp cut-off at 60 MeV

All 2qp states are included.

Calculation by Terasaki et al. (PRC71, 034310 (2005): Green line



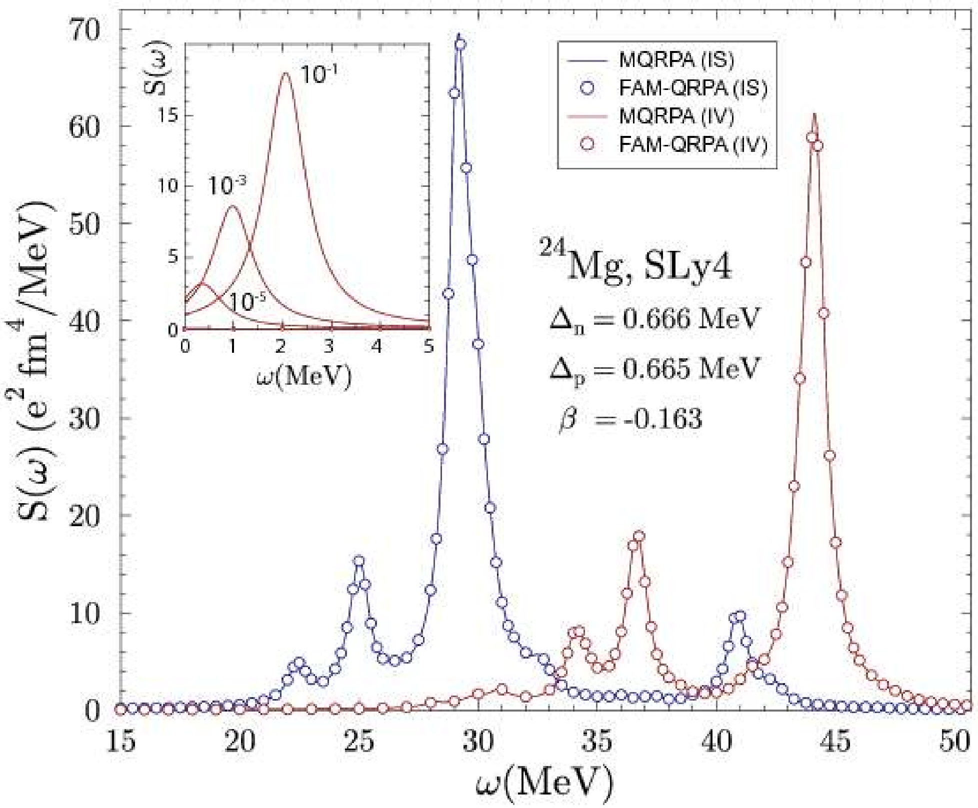
^{174}Sn, 0^+						
	$\omega = 4$ MeV		$\omega = 12$ MeV		$\omega = 20$ MeV	
η	ϵ	N_{iter}	ϵ	N_{iter}	ϵ	N_{iter}
10^{-2}	0.44	1000	$1.63 \cdot 10^{-1}$	1000	$8.84 \cdot 10^{-3}$	1000
10^{-4}	$6.10 \cdot 10^{-5}$	1000	$1.76 \cdot 10^{-5}$	1000	$< 10^{-5}$	469
10^{-5}	$< 10^{-5}$	161	$< 10^{-5}$	439	$< 10^{-5}$	469
10^{-8}	$< 10^{-5}$	161	$< 10^{-5}$	439	$< 10^{-5}$	469
10^{-9}	$< 10^{-5}$	161	$< 10^{-5}$	439	$< 10^{-5}$	469
10^{-10}	$< 10^{-5}$	161	$1.19 \cdot 10^{-5}$	1000	$1.46 \cdot 10^{-5}$	1000

Linearization parameter

$$\eta = 10^{-9} \sim 10^{-5}$$

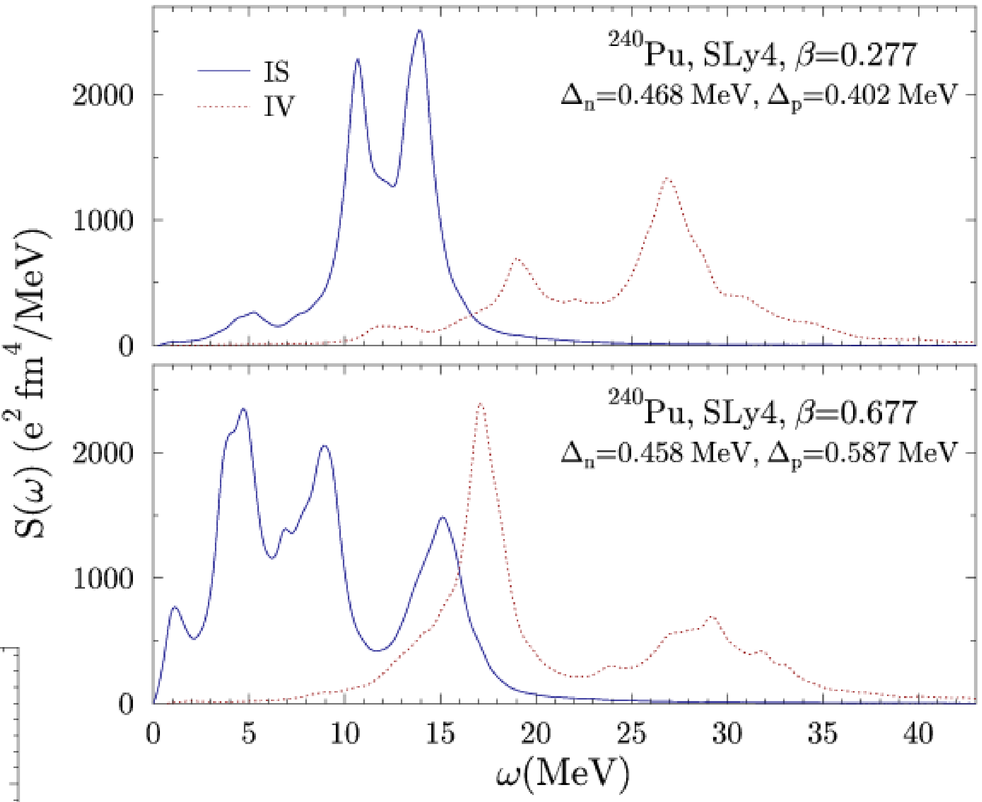
HFBTHO+FAM

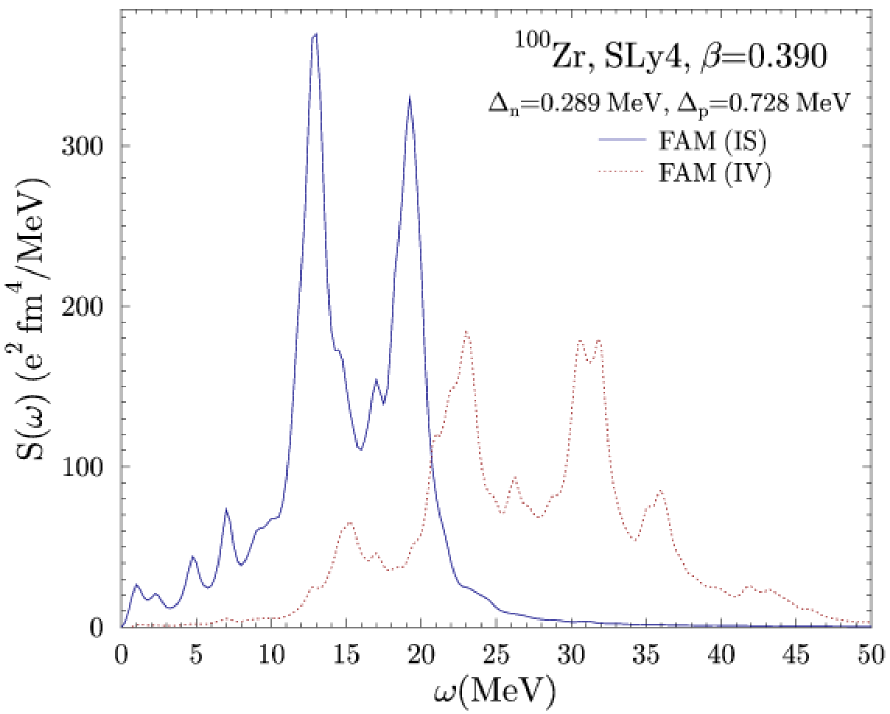
- N_{shell}=5
  - Comparison with Losa et al. PRC 81 (2010) 064307
- N_{shell}=20
  - Required memory sizes



QRPA			FAM
v_{crit}	Size of A, B matrices	Memory (in GB)	Memory (in GB)
^{40}Mg			
10^{-3}	32039×32039	16.4	
10^{-4}	53386×53386	45.6	
10^{-5}	53823×53823	46.35	
10^{-10}	130936×130936	274.31	
10^{-15}	189271×189271	473.18	
10^{-20}	211159×211159	713.41	0.572
^{100}Zr			
10^{-3}	83970×83970	112.81	
10^{-4}	140229×140229	314.63	
10^{-5}	160633×160633	412.85	
10^{-10}	189500×189500	574.56	
10^{-15}	230274×230274	848.41	
10^{-20}	230304×230304	848.64	0.572

- Cal. with N_{shell}=20
  - ^{100}Zr
  - ^{240}Pu (g.s. & f.i.)
  - Calculation was performed on a laptop PC.

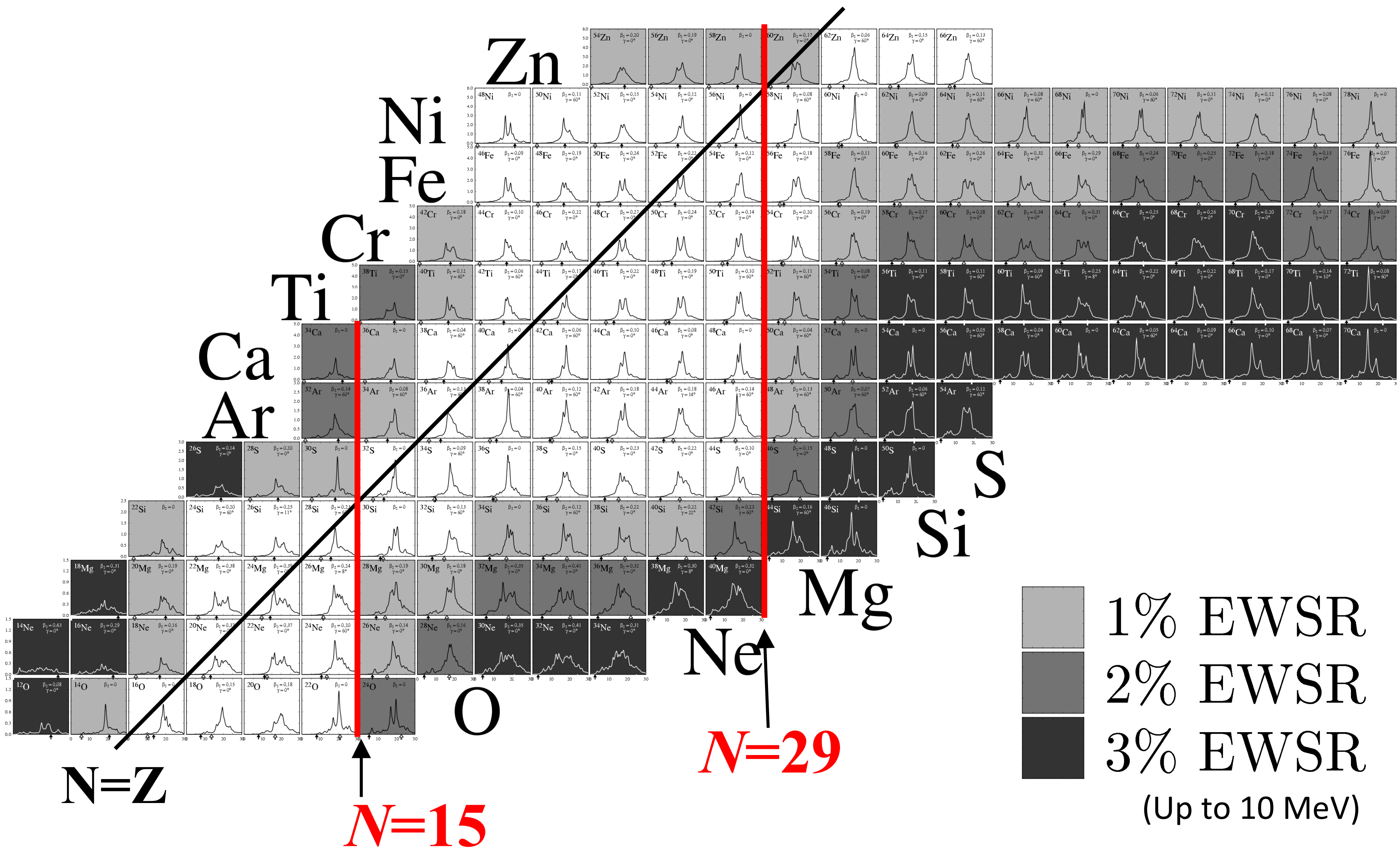




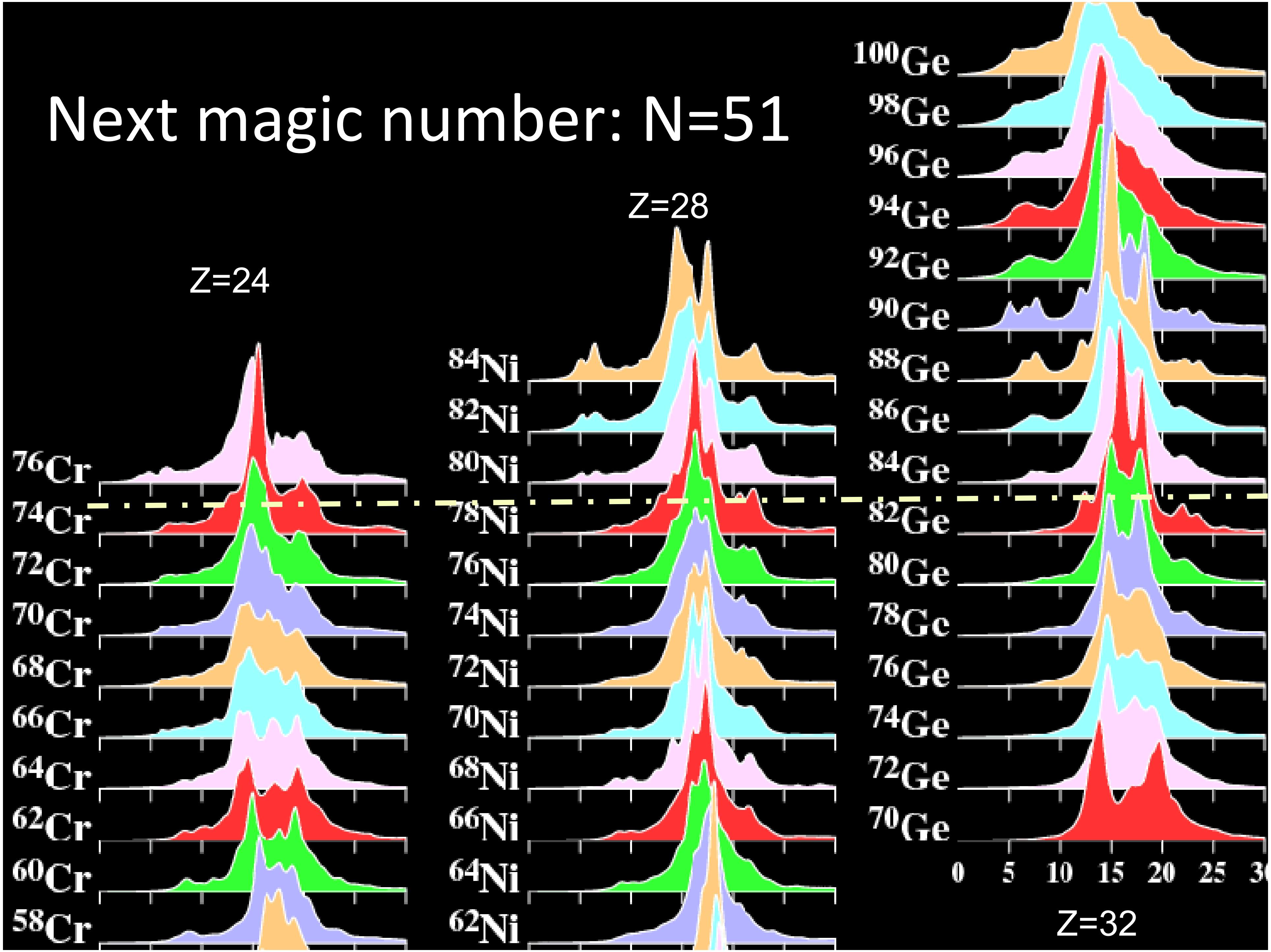
Pygmy dipole resonance (PDR)

- Inakura, T.N., Yabana, PRC in press, arXiv:1106.3618
  - Strong neutron shell effects
  - Correlation with neutron skin thickness

Magic numbers for PDR emergence

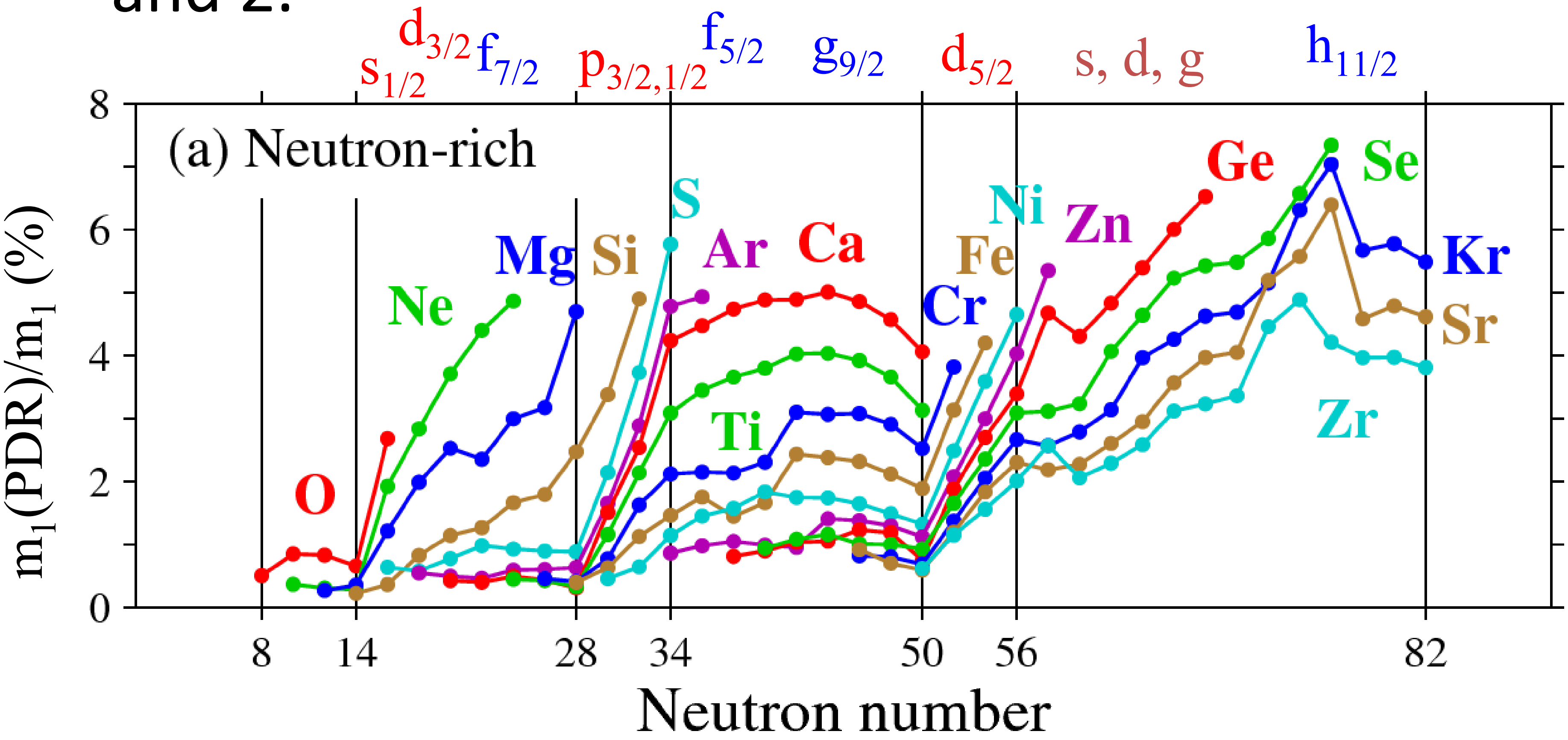


Next magic number: N=51



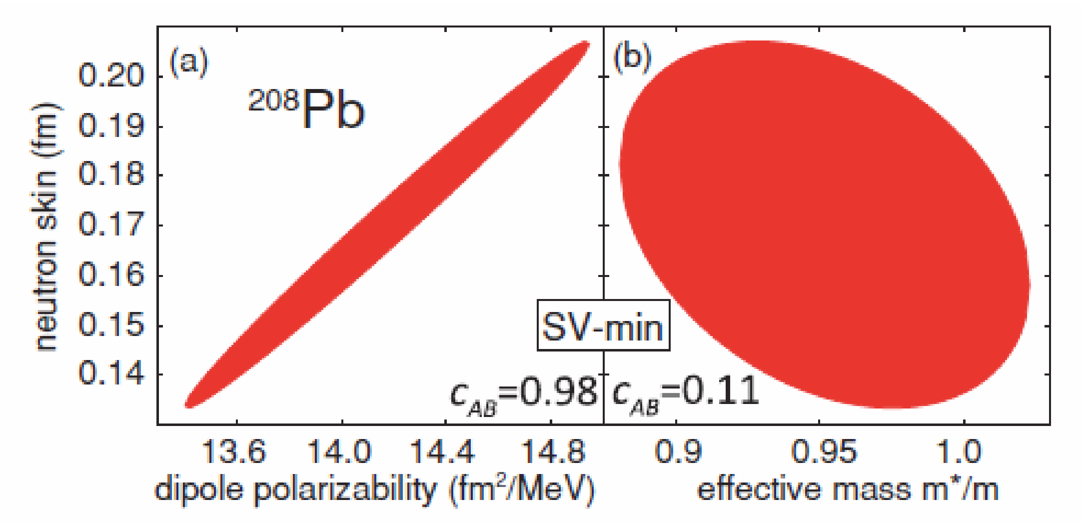
Magic numbers and low-l orbits

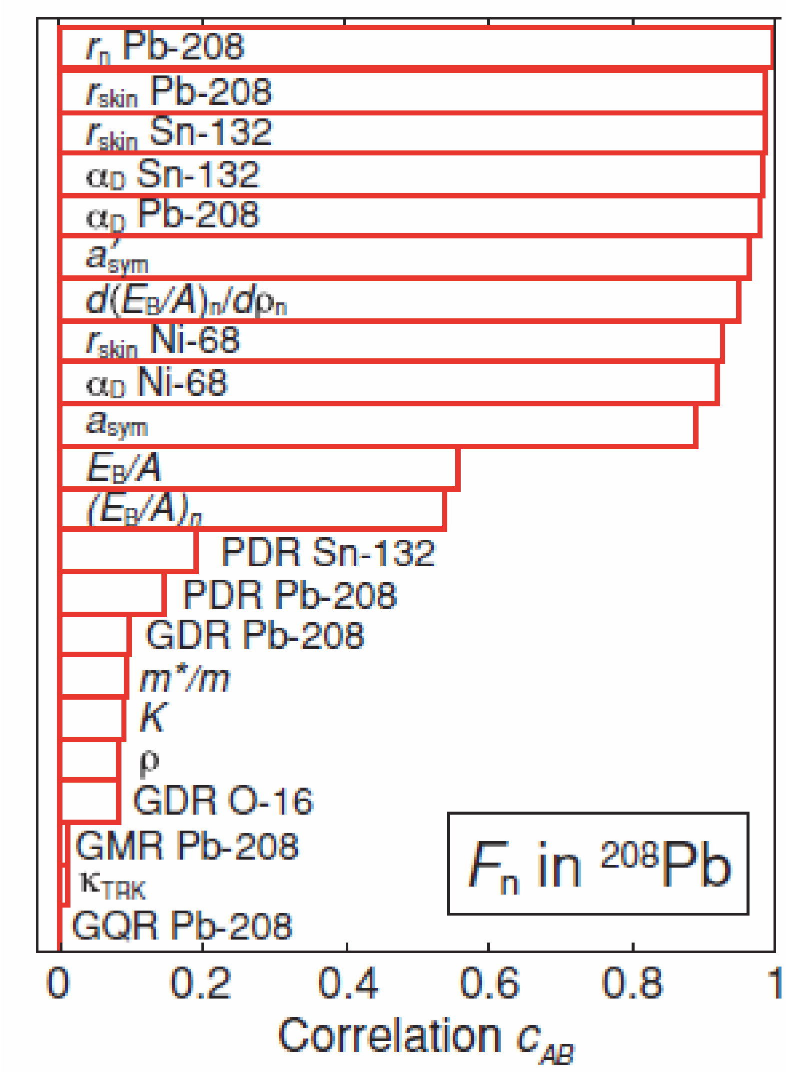
- Magic numbers: N=15, 29, 51, …
- Importance of weakly bound orbits with l=0, 1, and 2.



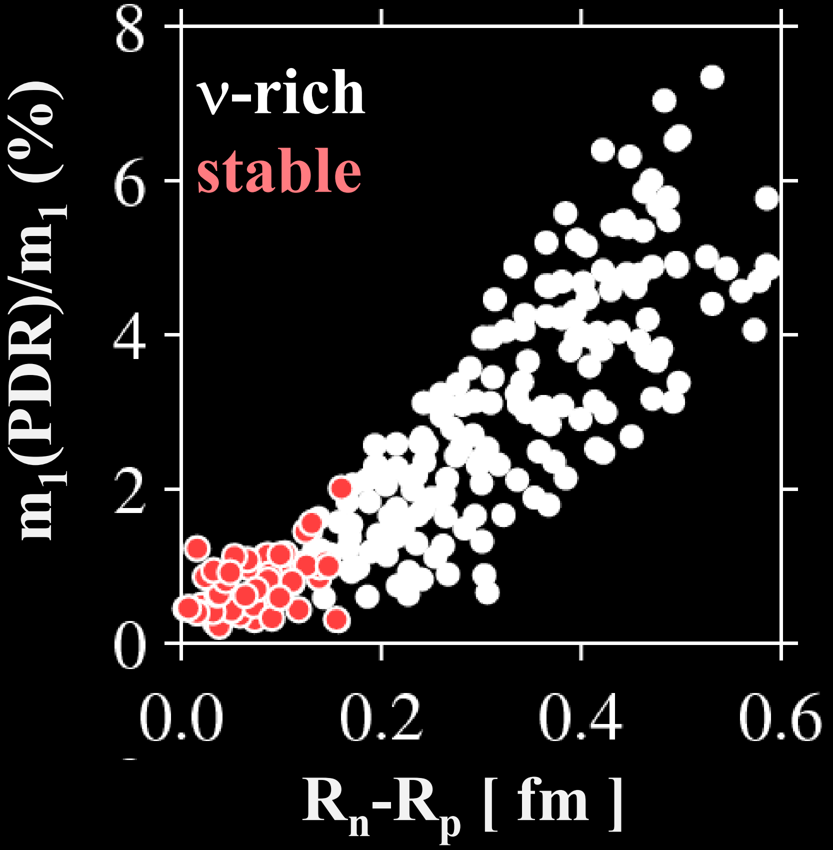
Pygmy dipole resonance (PDR) and neutron skin skinthickness

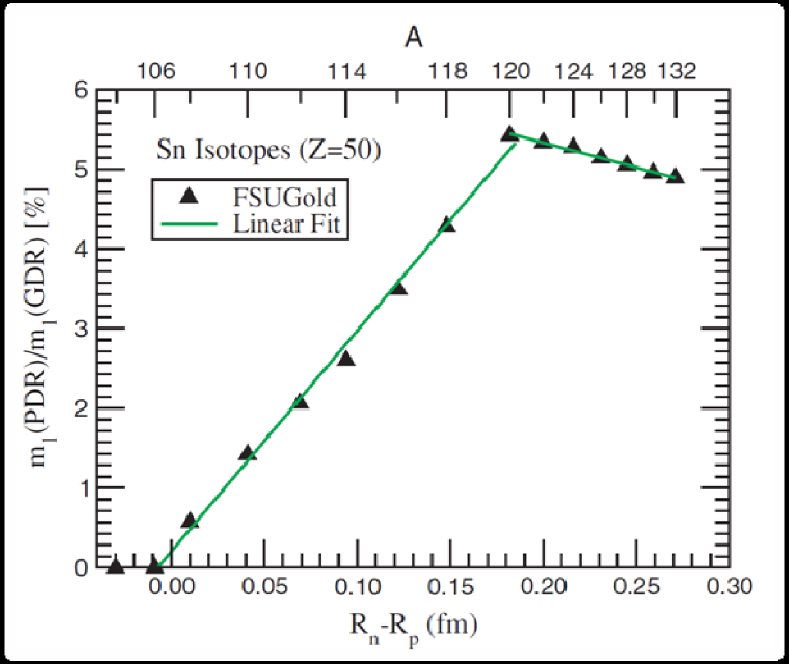
- Inakura, T.N., Yabana, PRC in press, arXiv:1106.3618
- Reinhard and Nazarewicz, PRC 81, 051303 (2010)
  - Ver weak correlation between PDR and neutron skin thickness





PDR strength vs neutron skin thickness



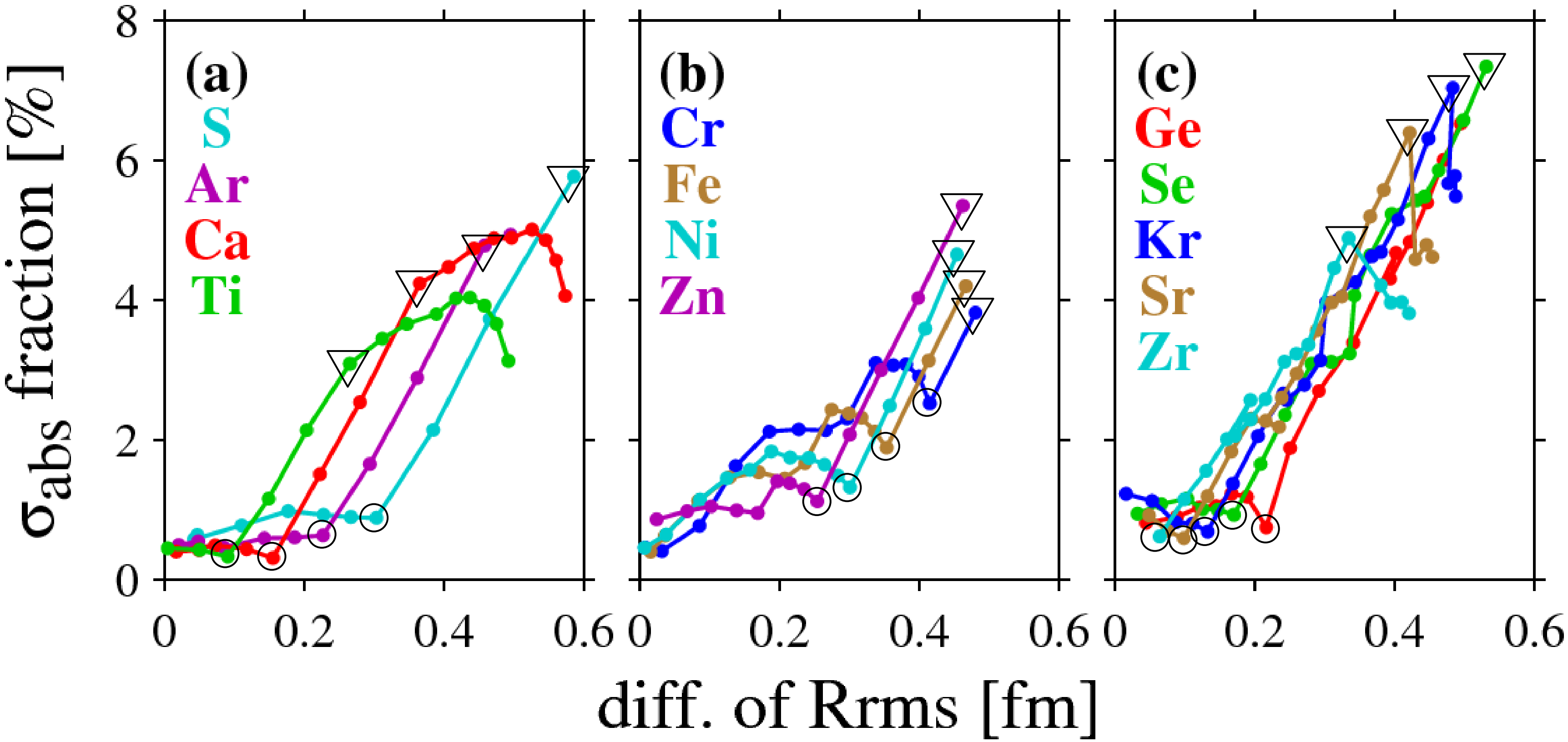


Piekarewicz, PRC73 (2006) 044325.

Weak correlation
(consistent with P.-G.&Witek, PRC81)

Universal correlation with skin thickness

- PDR fraction/ ΔR_{np} shows a universal rate, but for specific ranges of neutron numbers
- The rate is about 0.2 /fm.

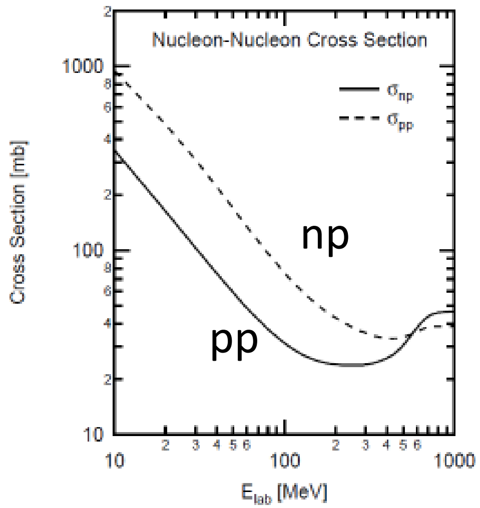


Reaction cross section in Glauber theory

Reaction cross section : $$\sigma_{\mathrm{R}} = \int db \left(1 - \left|e^{i\chi(\boldsymbol{b})}\right|^2\right),$$

Phase shift function: $$e^{i\chi(\boldsymbol{b})} = \langle \Psi_0 \Theta_0 | \prod_{i \in \mathrm{P}} \prod_{j \in \mathrm{T}} \{1 - \Gamma_{NN}(\boldsymbol{s}_i - \boldsymbol{t}_j + \boldsymbol{b})\} | \Psi_0 \Theta_0 \rangle.$$

Many-body operator, multiple integral

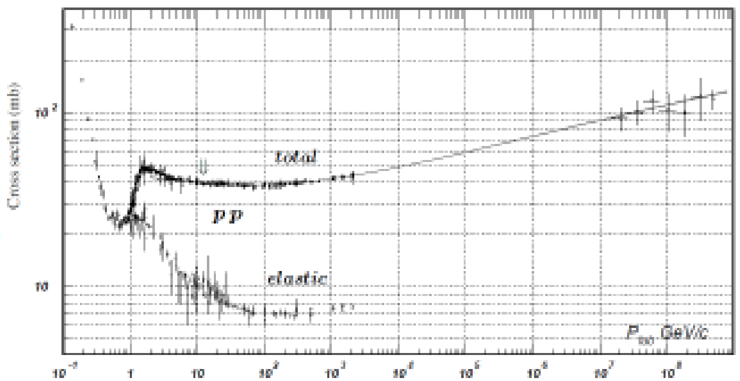


Profile function: $$\Gamma_{NN}(\boldsymbol{b}) = \frac{1 - i\alpha}{4\pi\beta} \sigma_{NN}^{\mathrm{tot}} \exp\left(-\frac{b^2}{2\beta}\right)$$

Parameters are fitted to reproduce N-N scattering

α : ratio of the real and imaginary part of the N-N scattering

β : slope parameter of the N-N elastic differential cross sections. Give a "range" of the interaction.



E < Pion production threshold $$\beta = \frac{1 + \alpha^2}{16\pi} \sigma_{NN}^{\mathrm{tot}}$$

E > Pion production threshold $$\sigma_{\mathrm{el}}^{\mathrm{NN}} = \frac{1 + \alpha^2}{16\pi\beta^2} \left(\sigma_{\mathrm{tot}}^{\mathrm{NN}}\right)^2$$

Practical way to calculate phase-shift function

$$G(\boldsymbol{b},\lambda) = \langle\Phi_0|\prod_{i=1}^{A}\left[1-\lambda\Gamma(\boldsymbol{b}-\boldsymbol{s}_i)\right]|\Phi_0\rangle$$

Need
λ =1

Cumulant expansion

$$\ln G(\boldsymbol{b},\lambda) = \lambda\left[\frac{\partial}{\partial\lambda}\ln G(\boldsymbol{b},\lambda)\right]_{\lambda=0} + \frac{1}{2}\lambda^2\left[\frac{\partial^2}{\partial\lambda^2}\ln G(\boldsymbol{b},\lambda)\right]_{\lambda=0} + \dots,$$

$$\left[\frac{\partial}{\partial\lambda}\ln G\right]_{\lambda=0} = -\langle\Phi_0|\sum_{i=1}^{A}\Gamma(\boldsymbol{b}-\boldsymbol{s}_i)|\Phi_0\rangle = -\int d\boldsymbol{r}\,\rho(\boldsymbol{r})\Gamma(\boldsymbol{b}-\boldsymbol{s})$$

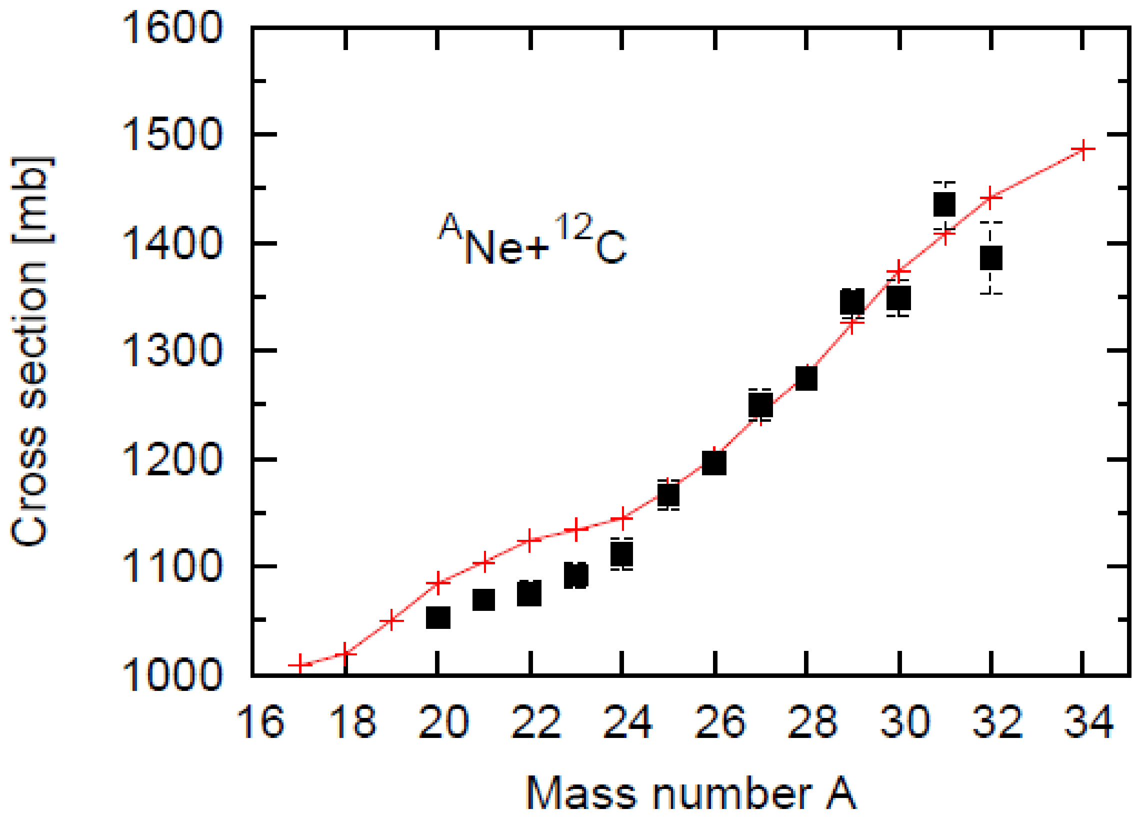
OLA: Optical Limit Approximation

$$\mathrm{e}^{i\chi_{\mathrm{OLA}}(\boldsymbol{b})} = \exp\left\{-\iint d\boldsymbol{r}d\boldsymbol{r}'\rho_{\mathrm{P}}(\boldsymbol{r})\rho_{\mathrm{T}}(\boldsymbol{r}')\Gamma_{NN}(\boldsymbol{s}-\boldsymbol{t}+\boldsymbol{b})\right\}$$

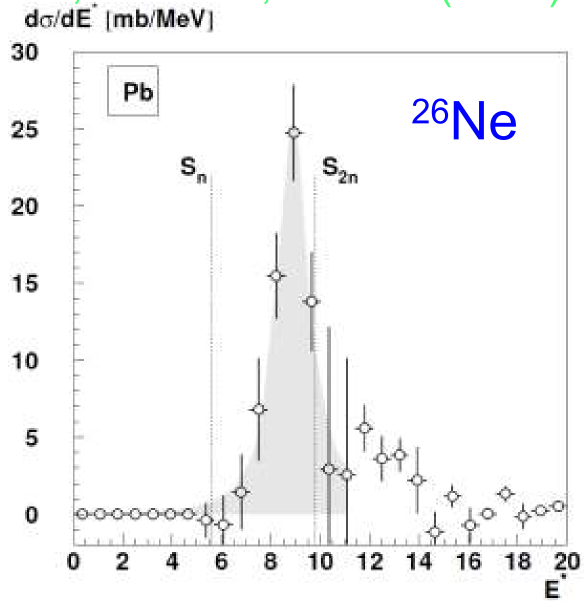
One-body density distributions are calculated by the 3D HF calculation.

Odd-A nuclei are calculated with the filling approximation.

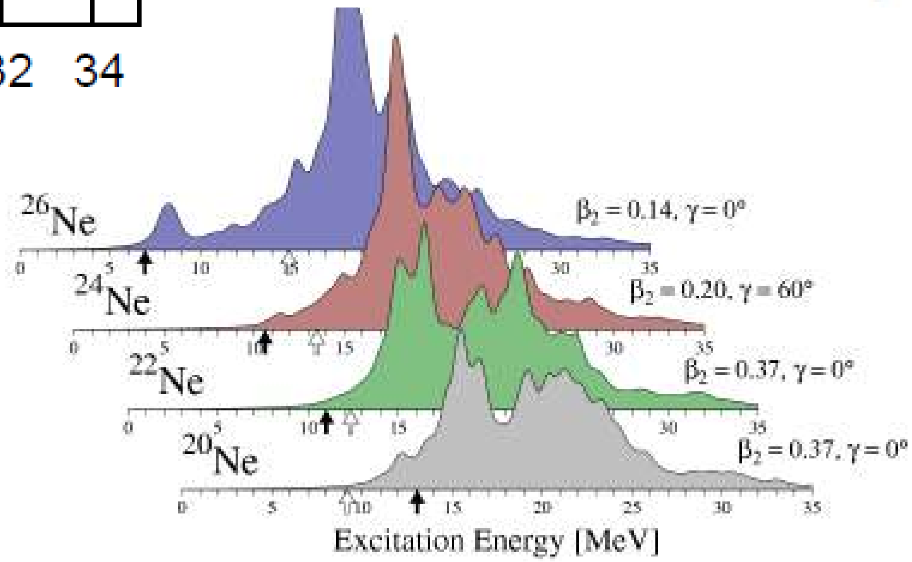
Ne isotopes at 240AMeV



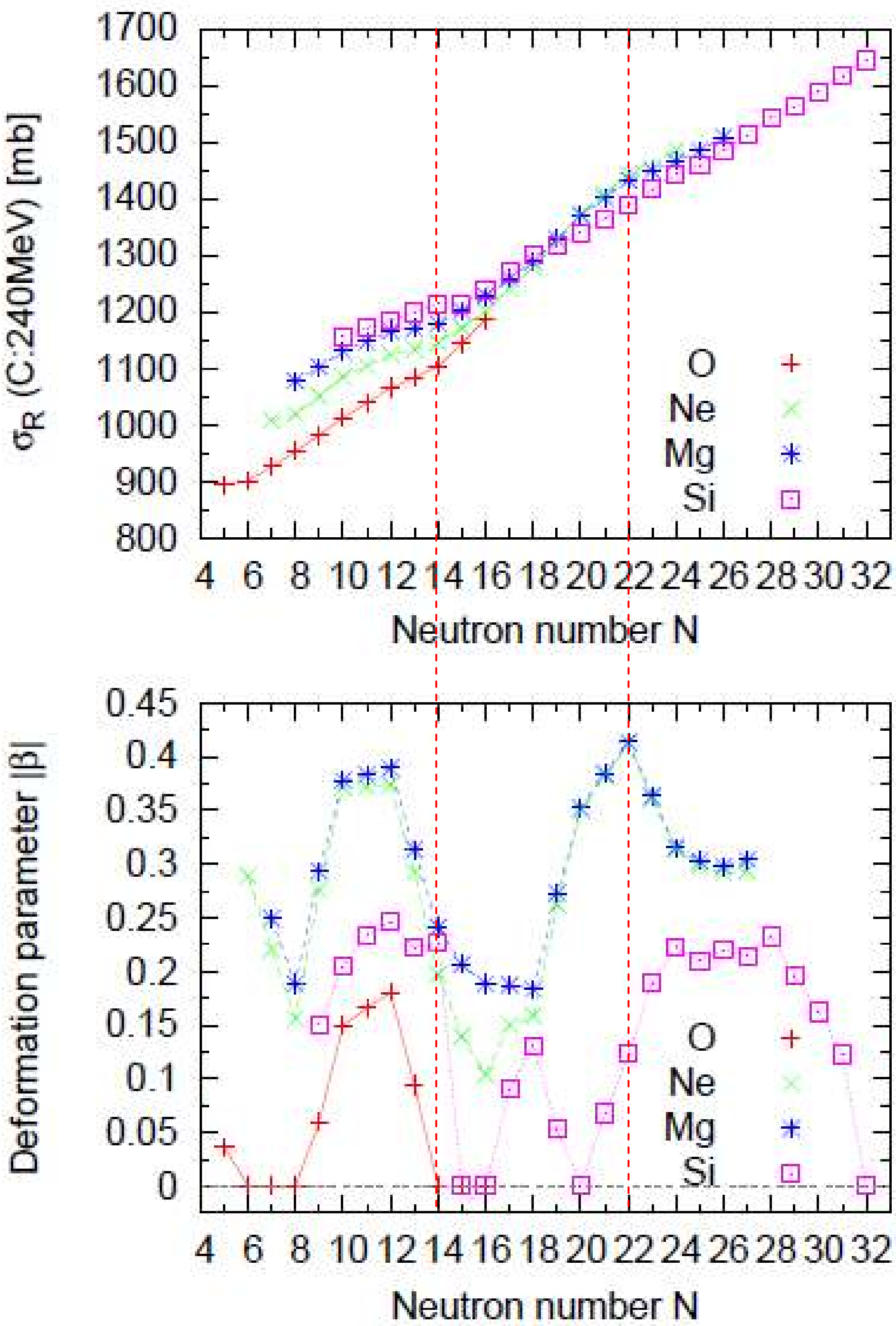
Gibelin et al, PRL 101, 212503 (2008)

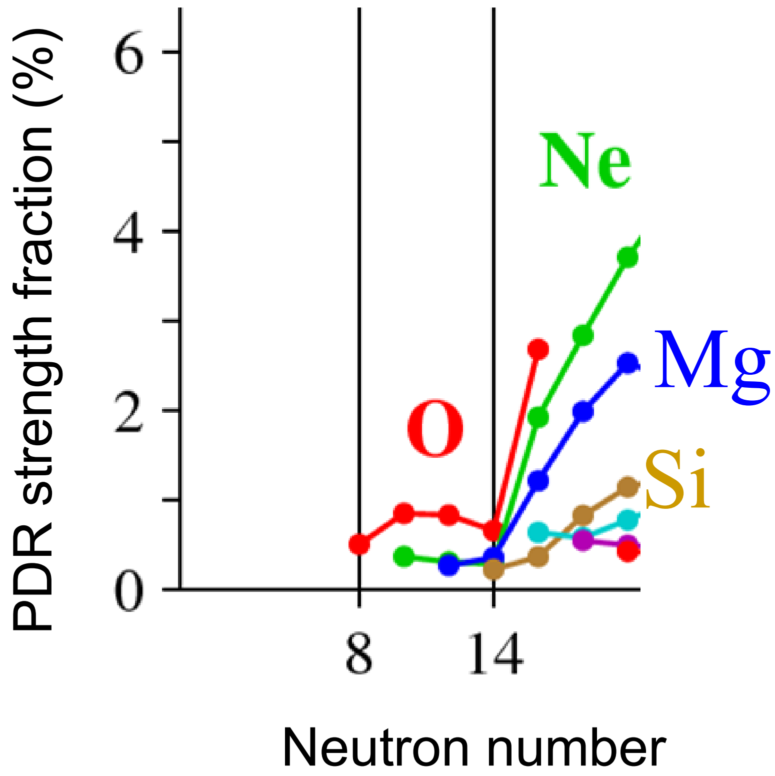


Exp: M. Takechi et al.,
Mod. Phys. Lett. A25, 1878 (2010).



Mean-field calculation for density provides a reasonable agreement, except for even-odd effects.





Kinks in σ_R and in PDR strength are due to s-wave contribution.

Deformation effect is seen in σ_R.

Summary

- Finite amplitude method (FAM) provides an alternative feasible approach to linear response calculation.
  - Several codes developed (FAM on 1D-, 2D-HFB, 3D-HF)
  - Systematic analysis on Pygmy Dipole Resonance (PDR)
    - Magic numbers for PDR (N=15, 29, 51, …), which are related to the occupation of low-*l* orbitals (*s, p, d*).
    - Universal correlation between the PDR fraction and the neutron skin thickness; $m_1(\mathrm{PDR})/m_1 \approx (0.2\ /\ \mathrm{fm})\,\Delta R_{np}$.
- Systematic calculations of reaction cross sections for O, Ne, Mg, Si isotopes
  - Qualitative agreement with experimental data
  - The kink at N=14 is consistent with that in PDR fraction

Collaborators

Paolo Avogadro (RNC/Milano), Shuichiro Ebata (RNC),
Tsunenori Inakura (RNC), Kazuhiro Yabana (Tsukuba/RNC)

Wataru Horiuchi (RNC), Yasuyuki Suzuki (Niigata/RNC),

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RNC: RIKEN Nishina Center (Wako, Japan)

ORNL: Oak Ridge Nat. Lab. (Oak Ridge, USA)

UTK: Univ. Tennessee (Knoxville, USA)

SISSA: Scuola Internazionale Superiore di Studi Avanzati (Trieste, Italy)